

2-Nitrobutane
600-24-8 | DTXSID3020968

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -39.7 °C

Global applicability domain: Inside

Local applicability domain index: 9.38e-01

Confidence level: 3.69e-01

Nearest Neighbors from the Training Set

Image not found

Propane, 2-methyl-1-nitro-

Measured: -76.9

Predicted: -40.3

Image not found

1-Nitrobutane

Measured: -81.3

Predicted: -46.4

Image not found

Propane, 2-methyl-2-nitro-

Measured: 26.2

Predicted: -20.5

Image not found

3-Methyl-1-nitrobutane

Measured: 97.0

Predicted: 31.6

Image not found

2-Nitropropane

Measured: -91.3

Predicted: -84.6